Scaling of the localization length in linear electronic and vibrational systems with long-range correlated disorder

Stefanie Russ

Institut für Theoretische Physik III, Universität Giessen, D-35392 Giessen, Germany (February 1, 2008)

The localization lengths λ of one-dimensional disordered systems are studied for electronic wavefunctions in the Anderson model and for vibrational states. In the first case, the site energies ϵ and in the second case, the fluctuations of the vibrating masses m at distance ℓ from each other are long-range correlated and described by a correlation function $C(\ell) \sim \ell^{-\gamma}$ with $0 < \gamma \le 1$. In the Anderson model, we focus on a scaling theory that applies close to the band edge, i.e. at energies E close to 2. We show that λ can be written as $\lambda = \lambda_0 f_{\gamma}(x)$, with $\lambda_0 = \langle \epsilon^2 \rangle^{-1/(4-\gamma)} \sim \lambda(E=2, \langle \epsilon^2 \rangle)$, $x = \lambda_0^2(2-E)$ and the scaling function $f_{\gamma}(x) = \text{const}$ for $x \ll 1$ and $f_{\gamma}(x) \sim x^{(3-\gamma)/2}$ for $x \gg 1$. Mapping the Anderson model onto the vibrational problem, we derive the vibrational localization lengths for small eigenfrequencies ω , $\lambda \sim \langle m \rangle^{(3-\gamma)/2} \langle m^2 \rangle^{-1} \omega^{-(1+\gamma)}$, where $\langle m \rangle$ is the mean mass and $\langle m^2 \rangle$ the variance of the masses. This implies that, unexpectateley, at small ω , λ is larger for uncorrelated than for correlated chains.

I. INTRODUCTION AND MODELS

A large amount of work has been done in the past decades to understand localization behavior in randomly disordered chains. Most work has been concentrated on uncorrelated [1] and short-range correlated disorder (see [2] and references therein). In this work, the effect of power-law long-range correlated disorder on the localization properties of linear electronic and vibrational systems is discussed.

First we consider the Schrödinger equation of a single-particle electronic wavefunction in tight binding approximation (Anderson model) [3],

$$\psi_{n+1} + \psi_{n-1} - 2\psi_n = -(2 - E + \epsilon_n)\psi_n. \tag{1}$$

Here E is the energy and $|\psi_n|^2$ is the probability to find an electron at site n, with $n \in \{1, N\}$. The ϵ_n are the site potentials and are random numbers, taken from an interval of width Δ , $\epsilon_n \in [-\Delta/2, \Delta/2]$ (diagonal disorder). $\langle \epsilon^2 \rangle \equiv (1/N) \sum_{n=1}^N \epsilon_n^2$ is their variance and the average value $\langle \epsilon \rangle \equiv (1/N) \sum_{n=1}^N \epsilon_n$ is zero. The term $-2\psi_n$ on both sides is introduced for technical reasons.

Second, we investigate the related problem of the localization length of vibrational states in disordered chains. In this case, the wavefunction ψ_n of Eq. (1) is substituted by the vibrational amplitudes u_n of N particles at sites n, coupled by unit spring constants between them. This problem is described by the time-independent eigenvalue equation with the vibrational amplitudes u_n and the eigenfrequencies ω :

$$u_{n+1} + u_{n-1} - 2u_n = -m_n \omega^2 u_n \tag{2}$$

Contrary to the ϵ_n of Eq. (1), all masses m_n are positive and taken from an interval $m_n \in [\langle m \rangle - \Delta/2, \langle m \rangle + \Delta/2]$, where $\langle m \rangle \equiv (1/N) \sum_{n=1}^N m_n > 0$ is their mean value and $\langle m^2 \rangle \equiv (1/N) \sum_{n=1}^N (m_n - \langle m \rangle)^2$ the variance.

The localization length λ in the Anderson case is defined by the exponential decay of the wavefunctions ψ_n , $\lim_{n\to\infty} |\psi_n/\psi_0| = \exp[-n/\lambda]$. In the vibrational problem, ψ_n/ψ_0 is substituted by u_n/u_0 , which decays accordingly.

In the standard Anderson model with uncorrelated diagonal disorder it has been recognized since long that in d=1 all states are exponentially localized [1,4,5], i.e., that λ approaches a constant for large N. A weak disorder expansion yields $\lambda = \langle \epsilon^2 \rangle^{-1/3} f((2-E)/\langle \epsilon^2 \rangle^{2/3})$ close to the band edge [6,7], while at the band center, a Green's function technique yields $\lambda \sim \langle \epsilon^2 \rangle^{-1}$ [8]. In some distance from the band center, the diagonal elements of the Green's functions can be developed by a second-order perturbation theory, yielding $\lambda(E) \sim (4-E^2)/\langle \epsilon^2 \rangle$ [9].

In the related vibrational problem with uncorrelated random masses, it is well accepted that all states in d=1 are localized, except for the case $\omega=0$, where the disorder term $m_n\omega^2$ disappears. Transfer matrix calculations in d=1 yield $\lambda\sim\omega^{-2}$ for small ω [10].

Here, we concentrate on long-range correlated disorder, characterized by a correlation function $C(\ell) \sim \ell^{-\gamma}$. In the Anderson case, $C(\ell)$ describes the correlations between site energies ϵ_n and $\epsilon_{n+\ell}$ at sites n and $n+\ell$,

$$C(\ell) = \lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^{N} \epsilon_n \epsilon_{n+\ell} \equiv \langle \epsilon_n \epsilon_{n+\ell} \rangle \sim \ell^{-\gamma} \quad (3)$$

with the correlation exponent $\gamma, 0 < \gamma \le 1$. In the vibrational problem, the mass fluctuations are long-range correlated and described by $C(\ell) = \langle \tilde{m}_n \tilde{m}_{n+\ell} \rangle \equiv \ell^{-\gamma}$ with $\tilde{m}_n \equiv m_n - \langle m \rangle$. The case $\gamma \ge 1$ describes only short-range correlated potentials. From random walk theory, we expect that series with $\gamma \ge 1$ fall into the same universality class as uncorrelated potentials [11,12].

For the one-dimensional Anderson model of Eq. (1) with long-range correlated potentials, a scaling form for the localization length $\lambda(E, \langle \epsilon^2 \rangle)$ close to the band edge E=2 has been developed recently and supported by preliminary numerical simulations [13]. For the vibrational problem, the localization length in the presence of correlations has not been adressed yet. In this paper, we determine explicitely the scaling function for the Anderson system and derive its asymptotic form by scaling arguments (section II). This leads also to an explicit expression for λ at intermediate energies in some distance from the band edge (cf. Eq.(10)). In section III, we map the Anderson model onto the vibrational problem and show that for small ω , $\lambda(\omega) \sim \omega^{-(1+\gamma)}$ which agrees with the result $\lambda \sim \omega^{-2}$ of [10] for random uncorrelated potentials, if we describe them by $\gamma = 1$. Accordingly, contrary to the expectations, λ is decreased by the presence of long-range correlations for $\omega \to 0$.

II. THE LONG-RANGE CORRELATED ANDERSON MODEL

In a previous work [13], it was shown by a space-renormalization procedure that at the band edge, E=2, the localization length λ scales as

$$\lambda(E=2,\langle\epsilon^2\rangle) \sim \langle\epsilon^2\rangle^{-1/(4-\gamma)} \equiv \lambda_0,$$
 (4)

For E < 2, but still in the neighborhood of 2, λ depends on both, λ_0 and 2 - E and can be written as:

$$\lambda(E, \langle \epsilon^2 \rangle) = \lambda_0 \ f_{\gamma}(x), \tag{5}$$

where
$$x = \lambda_0^2 (2 - E) = (2 - E) \langle \epsilon^2 \rangle^{-2/(4 - \gamma)}$$
 (6)

and $f_{\gamma}(x)$ is a correction function that depends on γ and approaches a constant for $x \to 0$. For $\gamma = 1$, one recovers the exponent $1/(4-\gamma) = 1/3$, in accordance with the result of [7] for uncorrelated potentials.

We are interested in the behavior of $f_{\gamma}(x)$ in the limits of large and small values of x. For uncorrelated potentials ϵ_n , we know already that $f_{\text{uncorr}}(x) \to \text{const}$ for $x \ll 1$ [7] and $f_{\text{uncorr}}(x) \to x$ for $x \gg 1$ [8,9]. We therefore assume a power-law behavior

$$f_{\gamma}(x) \sim x^{\alpha}$$
 (7)

for correlated potentials, where α depends on γ .

To derive the exponent α , it is helpful to realize that 1/(2-E) is proportional to the square of the wavelength Λ of the electronic wavefunction ($\langle \epsilon \rangle = 0$),

$$\Lambda^2 \sim 1/(2 - E). \tag{8}$$

This can be seen most easily in an ordered chain, where all $\epsilon_n=0$ and Eq. (1) reduces to $\psi''(x)/\psi(x)=-(2-E)$. The solution is a harmonic function with the wavelength Λ . In the case of disorder, we have calculated many states of correlated and uncorrelated chains

in different disorder intervals Δ by the Lanczos algorithm and have verified by Fourier transformation that relation (8) still holds. So, Λ describes the oscillating part of the wavefunction, while λ describes the exponential decay of the envelope. A similar relation for the wavelength has been found for vibrations in percolation clusters in d=2 and d=3 in [14].

Next, we look at a wavefunction with a given wavelength Λ and discuss, how λ is influenced by a change of the variance of the potentials $\langle \epsilon^2 \rangle$, i.e. by a change of λ_0 . We discuss the cases $x \ll 1$ and $x \gg 1$ separately, which correspond to $\Lambda \gg \lambda_0$ and $\Lambda \ll \lambda_0$, respectively. We have to keep in mind that Λ is solely determined by E, whereas λ_0 is determined by $\langle \epsilon^2 \rangle$ and γ .

- (i) For $\Lambda\gg\lambda_0$, close to the band edge, the wave amplitude decays within the first wavelength Λ . Accordingly, the wavefunction is independent of Λ and would not change for $\Lambda\to\infty$, i.e., by approaching the band edge, where $\lambda\sim\lambda_0\equiv\langle\epsilon^2\rangle^{-1/(4-\gamma)}$. Hence we expect for all γ that the scaling function $f_\gamma(x)=\lambda/\lambda_0$ approaches a constant for small x.
- (ii) In the opposite case, $\Lambda \ll \lambda_0$, the wave amplitude performs many oscillations before the envelope function decays completely. It is reasonable to assume that for the dependence of λ on the potential landscape, longrange correlations are not relevant, when the wavefunction oscillates rapidly. In this case, the term $\epsilon_n \psi_n$ on the right-hand side of Eq. (1) oscillates rapidly for both, correlated and uncorrelated potentials. So, in the case $\Lambda \ll \lambda_0$, we expect the same dependence of λ on $\langle \epsilon^2 \rangle$ for correlated and for uncorrelated potentials. For the latter, we know that in some distance from the band edge, the behavior of λ must cross over to the result of [9], $\lambda \sim \langle \epsilon^2 \rangle^{-1}$ and in view of the preceding remark, we expect the same behavior also for correlated potentials. Inserting this relation into (5) and (6), we find $f_{\gamma}(x) \sim x^{\alpha}$, with $\alpha = (3 - \gamma)/2$. In summary, we find for the asymptotic cases of the scaling function $f_{\gamma}(x)$ the power-law behavior

$$f_{\gamma}(x) \sim x^{\alpha} = \begin{cases} \text{const.} & x \ll 1\\ x^{(3-\gamma)/2} & x \gg 1 \end{cases}$$
 (9)

Inserting Eq. (9) into (5) and (6), we find for the energy dependence in the case $\Lambda \ll \lambda_0$ with the additional constraint $2-E \ll 1$

$$\lambda(E, \langle \epsilon^2 \rangle) \sim \langle \epsilon^2 \rangle^{-1} (2 - E)^{(3 - \gamma)/2}.$$
 (10)

Accordingly, we can distinguish between three energy regimes. (a) For $2-E\ll\langle\epsilon^2\rangle^{-2/(4-\gamma)}$, i.e., very close to the band edge, we have $\lambda\sim\langle\epsilon^2\rangle^{-1/(4-\gamma)}$, independent of E. (b) For $1\gg 2-E\gg\langle\epsilon^2\rangle^{-2/(4-\gamma)}$, Eq. (10) applies. (c) For still larger values of 2-E, the scaling behavior breaks down.

For growing values of 2-E, it was obtained that in some distance from the band center $\lambda(E) \sim (2-E)(2+E)/\langle\epsilon^2\rangle$ for uncorrelated potentials [9]. This expression emerges into Eq. (10), if we set $\gamma=1$, which yields $\lambda \sim (2-E)/\langle\epsilon^2\rangle$. So we can see again that the case of uncorrelated potentials is well described by $\gamma=1$.

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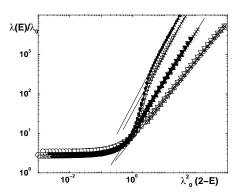


FIG. 1.: Plot of the scaling function $f_{\gamma}(x) = \lambda(E)/\lambda_0$ versus $x = \lambda_0^2 \, (2-E)$ close to band edge for the Anderson model in d=1. The curves show (from bottom to top): uncorrelated disorder (large open symbols), correlated site potentials of $\gamma=0.5$ (large filled symbols), $\gamma=0.1$ (small open symbols) and $\gamma=0.01$ (small filled symbols). The symbols stand for $2-E=10^{-4}$ (circles), 10^{-3} (squares), 10^{-2} (diamonds), 0.1 (triangles up), 0.2 (triangles down), 0.3 (x) and $\langle \epsilon^2 \rangle$ was varied between 10^{-5} and 10^{-1} . The typical average of λ was performed over 1000 chains of length $N=2^{20}$. The straight lines of the theoretical slopes $(3-\gamma)/2$ are guides to the eye.

In order to test this scaling function, we have generated $\nu=1000$ linear chains of size $N=2^{20}$ by the method of Fourier transformation [15] and calculated the individual localization lengths λ_i by the transfermatrix method [1,12,16]. To obtain the mean localization length, we performed the typical (logarithmic) average $\lambda(E,\langle\epsilon^2\rangle)\equiv\lambda_{\rm typ}=\exp[\frac{1}{\nu}\sum_{i=1}^{\nu}\ln\lambda_i]$.

To obtain the scaling function $f_{\gamma}(x)$, we plotted λ/λ_0 versus $x=\lambda_0^2\,(2-E)$. The results are shown in Fig. 1 for (from bottom to top) uncorrelated potentials (described by $\gamma=1$) and correlated potentials with $\gamma=0.5,0.1$ and 0.01. Five values of (2-E) between 10^{-4} and 0.3 were calculated while $\langle\epsilon^2\rangle$ varied between $\langle\epsilon^2\rangle=10^{-5}$ and 10^{-1} . The figure supports the scaling theory. The data for the different 2-E and $\langle\epsilon^2\rangle$ fall onto the same scaling functions $f_{\gamma}(x)$, which show the expected behavior (cf. Eq. (9)) in the asymptotic cases. The lines are guides to the eye with the theoretical slopes of $\alpha=(3-\gamma)/2$. A crossover close to x=1 separates the cases $x\ll 1$ and $x\gg 1$, i.e. $\lambda_0^2\ll 1/(2-E)$ and $\lambda_0^2\gg 1/(2-E)$. In the case $x\ll 1$, we find $\lambda/\lambda_0={\rm const}$, i.e. $\alpha=0$.

III. THE LONG-RANGE CORRELATED VIBRATIONAL MODEL

This scaling theory can be generalized to the vibrational problem, described by Eq. (2). We split m_n into the average part $\langle m \rangle$ and the fluctuation part \tilde{m}_n , $m_n = \langle m \rangle + \tilde{m}_n$ and can map the Anderson problem onto the vibrational problem by replacing

$$2 - E \to \omega^2 \langle m \rangle$$
 and $\epsilon_n \to \omega^2 \tilde{m}_n$. (11)

We obtain the wavelength $\Lambda \sim (\langle m \rangle^{1/2} \, \omega)^{-1}$ by inserting (11) into (8) and the scaling variable x by inserting (11) into (6), yielding (with $\langle \hat{m}^2 \rangle = \langle m^2 \rangle$)

$$x = \langle m \rangle \,\omega^{-2\gamma/(4-\gamma)} \langle m^2 \rangle^{-2/(4-\gamma)}. \tag{12}$$

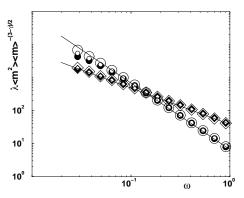


FIG. 2.: The scaled localization length $\lambda \langle m^2 \rangle \langle m \rangle^{-(3-\gamma)/2}$ for the vibrational chain is plotted versus the eigenfrequency ω for uncorrelated masses (circles) and correlated masses of $\gamma=0.1$ (diamonds) for different $\langle m \rangle$ and disorder intervals Δ : $\langle m \rangle=0.5$, $\Delta=0.99$ (large open symbols), $\langle m \rangle=0.5$, $\Delta=0.5$ (filled symbols) and $\langle m \rangle=0.25$, $\Delta=0.49$ (small open symbols). The values of $\Delta=0.99$ and 0.5 refer zu $\langle m^2 \rangle \approx 0.008$ and 0.002, respectiveley. The typical average of λ was performed over 1000 chains of length $N=2^{23}$. The lines with the slopes $1+\gamma$ are guides to the eye. Small deviations from the straight line at very large values of $\lambda \approx N/2$ are finite-size effects.

Since $\langle m^2 \rangle < \langle m \rangle^2$, we can easily verify that for $\omega^2 < 1/\langle m \rangle$, the scaling variable x is greater than 1. Therefore, contrary to the Anderson problem, we have only one scaling regime x>1. Inserting (11) into (10), we find λ for the vibrational problem:

$$\lambda \sim \langle m \rangle^{(3-\gamma)/2} \langle m^2 \rangle^{-1} \omega^{-(1+\gamma)}$$
. (13)

This relation is valid for small values of $\omega^2\langle m\rangle$. In our simulations, we found that for e.g. $\langle m\rangle=0.5$, it holds approximately for $\omega<1$. In order to test Eq. (13), we have calculated the typical average $\lambda_{\rm typ}$ of 1000 chains of length 2^{23} for different values of γ , $\langle m\rangle$ and $\langle m^2\rangle$ by the transfer-matrix method. In Fig. 2, the scaled localization length $\lambda \langle m^2\rangle \langle m\rangle^{-(3-\gamma)/2}$ is plotted versus ω for $\gamma=0.1$ and for uncorrelated random chains (described by $\gamma=1$). Both, the data collapse for chains of different $\langle m\rangle$ and $\langle m^2\rangle$ and the slopes support Eq. (13). The lines are guides to the eye with the theoretical slopes of $-(1+\gamma)$ and describe the behavior of λ very well.

Two phenomena are worth mentioning here. First, λ diverges if $\omega \to 0$. The reason is that the disorder term m_n in (2) appears only in combination with the eigenvalue ω^2 and therefore disappears for $\omega \to 0$. Second,

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for large ω , λ is larger for the correlated than for the uncorrelated chains. However, below some crossover frequency (that depends on γ), this behavior changes and the vibrational excitations of the correlated chains become more localized. This, at the first glance unexpected behavior can be understood as follows.

Large ω correspond to small wavelengths Λ . Particles m_n in distances less than $\Lambda/2$ from each other move into the same direction and can roughly be considered as an effective hyperparticle $M_j \sim \sum_{n=1}^\mu m_n$, where the sum runs over all μ particles in the region of the size of $\Lambda/2$. The effective disorder seen by the vibrational excitation depends on the distribution of the M_j in the region, where the wave amplitude is large. For strongly correlated chains, there exist large regions of masses m_n that are either below the average mass $\langle m \rangle$ or above. So, as long as $\Lambda/2$ is smaller than the size of these regions, the distribution of the M_j is more narrow for correlated than for uncorrelated chains, which leads to larger λ .

This behavior changes when the size of $\Lambda/2$ is well above the size of the correlated regions. Now, on scales of $\Lambda/2$ the system looks much more disordered than before. We know from random-walk theory that for large μ the variance of the M_j scales as $\sim \mu^{2-\gamma}$ [11]. Hence, for large μ the distribution M_j is broader in correlated than in uncorrelated chains and therefore, the disorder seen by the vibrational excitation is even larger. Therefore, we expect smaller λ for the correlated chains, when $\omega \to 0$.

The same effect appears also in the Anderson model, where, according to Eq. (10), λ is also smaller for correlated than for uncorrelated chains in the limit of small values of 2-E. For systems at the band edge, this has already been reported in [13].

IV. CONCLUSIONS

In summary, we have studied the effect of long-range correlated disorder on the localization lengths of electron states in the one-dimensional Anderson model and of the vibrational states of harmonic chains. In the Anderson model, the site potentials ϵ are long-range correlated, while in the vibrational problem we have long-range correlations in the fluctuation part \tilde{m}_n of the masses around their mean value $\langle m \rangle$.

First, we studied the scaling behavior of the localization length λ in the Anderson model close to the band edge E=2. We have shown that two characteristic lengths occur: the wavelength Λ that describes the oscillating part of the wavefunction and the localization length λ_0 that describes how the envelope of the wavefunction decays at the band edge. While Λ depends on the energy E, λ_0 depends on the variance $\langle \epsilon^2 \rangle$ and the correlation exponent γ . We developed a scaling theory, with the scaling variable $x=\lambda_0^2/\Lambda^2$. Using qualitative arguments, we derived the asymptotic behavior of the

scaling function, both, for $\Lambda \gg \lambda_0$ and $\Lambda \ll \lambda_0$, and thus the behavior of λ in these limits. It was found that λ is independent of E at very small values of 2-E. For larger distances from the band edge, but E still in the neighborhood of 2, it depends on 2-E and on $\langle \epsilon^2 \rangle$ by power-laws.

Second, we developed an analogous scaling theory for the vibrational problem by mapping the Anderson equation onto the equations of motion of harmonic vibrations. We found that $\lambda(\omega) \sim \omega^{-(1+\gamma)}$ in the limit of small frequencies and for $0 < \gamma \le 1$. This relation may constitute a possibility to measure correlations by determining the localization length of vibrations. It implies that λ grows faster for uncorrelated than for correlated chains, when $\omega \to 0$. This is in close analogy to the behavior of λ in the Anderson model at the band edge and arises from the coupling of correlated masses over very large distances, which leads to larger fluctuations than in the case of uncorrelated potentials. Accordingly, for very small frequencies, correlated chains have smaller localization lengths than uncorrelated ones.

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